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Novel Parallel Numerical Methods for Radiation & Neutron Transport

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DISCLAIMER

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LDRD Final Report

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PROJECT OVERVIEW

In many of the multiphysics simulations performed at LLNL, transport calculations can take up 30 to 50% of the total run time. If Monte Carlo methods are used, the percentage can be as high as 80%. Thus, a significant core competence in the formulation, software implementation, and solution of the numerical problems arising in transport modeling is essential to Laboratory and DOE research.

In this project, we worked on developing scalable solution methods for the equations that model the transport of photons and neutrons through materials. Our goal was to reduce the transport solve time in these simulations by means of more advanced numerical methods and their parallel implementations. These methods must be scalable, that is, the time to solution must remain constant as the problem size grows and additional computer resources are used. For iterative methods, scalability requires that (1) the number of iterations to reach convergence is independent of problem size, and (2) that the computational cost grows linearly with problem size.

We focused on deterministic approaches to transport, building on our earlier work in which we performed a new, detailed analysis of some existing transport methods and developed new approaches. The Boltzmann equation (the underlying equation to be solved) and various solution methods have been developed over many years. Consequently, many laboratory codes are based on these methods, which are in some cases decades old. For the transport of x-rays through partially ionized plasmas in local thermodynamic equilibrium, the transport equation is coupled to nonlinear diffusion equations for the electron and ion temperatures via the highly nonlinear Planck function. We investigated the suitability of traditional-solution approaches to transport on terascale architectures and also designed new scalable algorithms; in some cases, we investigated hybrid approaches that combined both.

TECHNICAL APPROACH

We next describe the solution approaches we pursued during this LDRD effort. Our methods all involved multilevel solution strategies. Briefly, the *First-Order System Least Squares* (FOSLS) solution approach to the Boltzmann equation is a new technique that is completely based on

multilevel methods. Our other solution approaches for the Boltzmann equation are hybrid in nature, combining traditional and mulitlevel methods. Our solution approaches for radiation-diffusion are fully implicit and nonlinear, and also utilize multilevel methods.

Boltzmann Solution Methods Based on FOSLS

FOSLS methods have been successfully applied to obtain uniformly fast and accurate solvers for some classes of applications involving High Reynolds flow, linear elasticity approaching the incompressible limit, and highly indefinite Helmholtz problems. One of the main advantages of FOSLS is its formulation as a *minimization principle* for problems that have no other natural optimization form. This leads to several benefits:

- discretization can be done via Rayleigh-Ritz techniques, which are simpler than Galerkin methods because they need only one type of subspace and more powerful because they can exploit the optimization structure;
- such 'variational' multigrid methods are typically more effective and better supported by theory than non-variational schemes;
- heuristics and analysis of discretization can be based on approximation theory instead of more cumbersome and often misleading approaches like truncation error analysis; and
- local and global *a posteriori* error measures in a meaningful norm are readily available.

An important use of local and global *a posteriori* error estimates is in performing adaptive mesh refinement in space and direction (angle). Another benefit of a FOSLS approach is the elimination of ray effects. Ray effects are often present when using discrete ordinates methods on problems with sources localized in space and/or highly anisotropic in direction (angle). As the FOSLS approach naturally utilizes a P_N approach to the directional (angular) discretization, ray effects can be eliminated.

Boltzmann Hybrid Solution Approaches

We now discuss other approaches we pursued that can be effective, and at the same time more easily fit into solution techniques currently being used. In earlier work, we devised an effective technique for eliminating ray effects in discrete ordinates transport codes. This approach, called *Harmonic Projection*, obtains a spherical harmonics solution to the Boltzmann equation (i.e., a solution to the related P_N system), and only requires a minor change to the existing discrete-ordinates solution procedure. We have successfully applied this technique to several problems, and we outline its use in a full system ASCI Blue SST run below. Another effective technique used in discrete ordinates methods is diffusion synthetic acceleration (DSA), a preconditioner based on solving a related diffusion problem. We developed a DSA preconditioner for our time dependent Boltzmann code that utilizies multigrid to solve the diffusion system.

Radiation-Diffusion Solution Approaches

For many years, we have actively developed parallel time-stepping solution methods for time-dependent partial differential systems. This work, funded by LDRD, has resulted in a suite of parallel solvers (called *PVODE*) for coupled time-dependent differential systems discretized using a semi-discretization approach in which only some phase space variables have been

discretized. This approach leads to solving systems of ordinary differential equations (ODEs), sometimes coupled to purely algebraic systems, i.e., differential/algebraic systems (DAEs). Typically, these systems are stiff, and so require an implicit treatment of the time discretization. The *PVODE* solver uses variable order timestepping algorithms and preconditioned Krylov iteration methods to solve the resulting linear systems. Many codes at the Laboratory use an operator splitting approach for timestepping, and can be limited in the size of the time step by accuracy and/or stability considerations. We have investigated the suitability of using the *PVODE* suite in solving coupled radiation and material energy transfer simulations. The major difficulty when using the *PVODE* solver is finding an effective preconditioner.

ACCOMPLISHMENTS

FOSLS Transport Solver Accomplishments

During the course of this project we developed a parallel FOSLS-based transport solver for the Boltzmann equation using a spherical harmonics directional discretization. An initial scalability study was performed using our parallel solver, with the results described in Table 1 below. The test problem used in the study had isotropic scattering with a total cross section σ_T and an absorption cross section σ_a as discussed in the caption using a 1cm on a side box for the spatial domain. Several different order P_N approximations were used. The number of nodes (or vertices) in the spatial grid varied. As the results indicate, our procedure scales very well, both in run time and iteration count. For very diffusive problems, our iterative solution method suffers a slowdown of the convergence rate, and our current research is focused on fixing this.

Table 1. Scalability Study for FOSLS Code: V-cycle results for two case studies of cross sections. For Problem 1, $\sigma_T = .1$ and $\sigma_a = .1$, while for Problem 2, $\sigma_T = 10$ and $\sigma_a = 5$.

					Problem 1		Problem 2	
P_N	Nodes	Unknowns	Procs	Unk/Proc	Iters	Time	Iters	Time
1	33^3	4×33^3	1	143,748	9	279	10	213
1	65^3	4×65^3	8	137,313	9	261	10	294
1	129^3	4×129^3	64	134,168	9	267	10	296
1	257^3	4×257^3	512	132,614	9	270	10	302
3	17^3	16×17^3	1	78,608	20	511	14	359
3	33^3	16×33^3	8	71,874	20	472	15	356
3	65^3	16×65^3	64	68,656	20	495	17	413
3	129^3	16×129^3	512	67,084	20	534	19	467
6	9^3	49×9^3	1	35,721	34	1,381	12	496
6	17^3	49×17^3	8	30,092	41	1,493	19	698
6	33^3	49×33^3	64	27,514	43	1,607	24	903
6	65^3	49×65^3	512	26,282	45	1,743	29	1,142

6	17^3	49 x 17^3	1	240,737	40	9,224	20	4,591
6	129^3	49 x 129^3	512	205,444	47	10,191	30	6,320
9	9^3	100 x 9^3	1	72,900	50	8,791	14	2,406
9	17^3	100 x 17^3	8	61,413	65	9,757	26	3,979
9	33^3	100 x 33^3	64	56,152	71	10,798	37	5,652
9	65^3	100 x 65^3	512	53,637	74	11,468	45	7,047

Radiation-Diffusion Solver Accomplishments

We developed a parallel 3D fully implicit solution technique based on *PVODE* for the coupled nonlinear system of equations involving the energy and electron densities modeling radiation-diffusion. This work uses parallel Newton-Krylov/multigrid solvers for the solution of the nonlinear equations at each time step. Our code is also capable of using a multigroup approximation in energy or solves instead an integrated in energy form of the radiation-diffusion equations. We performed a scalability study of our integrated in energy radiation-diffusion code on ASCI Red going up to 5,832 processors. The problem used Planck and Rosseland opacity values that were constant, equal and set to the value 10^5. This problem was run to a final time of 10^{-2}s. A grid of 40x40x40 was used on each processor, and the problem was scaled form 1 to 5,832 ($=18^3$) processors giving a total of 746,496,000 unknowns in the largest problem. Table 2 shows the solver statistics for this study. We see that the number of time steps, as well as the number of nonlinear and linear iterations scale very well. In addition, the run time scales extremely well with 83% scaled efficiency for the 5,832 processor run. The run time per time step also scales very well at about 75% scaled efficiency for 5,832 processors.

Table 2. Solution statistics for the integrated in energy radiation diffusion model with constant opacity values using a 40^3 grid per processor.

Topology	#Unknowns	Run Time (s)	# Time Steps	# Nonlin.	# Lin. Its.
1x1x1	128,000	2,485	123	140	186
2x2x2	1,024,000	2,518	113	127	160
4x4x4	8,192,000	2,424	105	119	154
8x8x8	65,536,000	2,761	119	136	191
16x16x16	524,288,00	2,970	116	129	212
18x18x18	746,496,00	3,001	112	130	214

We also performed a scaled efficiency study on the ASCI Blue machine utilizing 1,024 processors. For this case, opacities from the LEOS equation of state package were used with the material carbon. Table 3 shows the solver statistics and run times for this study. Here, we see about 56% scaled efficiency of the time steps at 1,024 processors. Again, we see good algorithmic scalability of the nonlinear and linear iterations. The simulation was run to about 0.001 microseconds.

Table 3. Solution statistics for the integrated in energy radiation diffusion model with tabulated opacity values using a 40^3 grid per processor.

Topology	# Unknowns	Run Time	# Time Steps	# Nonlin.	# Lin. Its.
1x1x1	128,000	2,015	217	329	423
2x2x2	1,024,000	2,287	214	324	411
4x4x4	8,192,000	2,220	196	295	378
8x8x8	65,536,000	2,575	197	273	374
16x8x8	131,072,000	3,106	190	273	376

We developed, analyzed and compared four different preconditioning strategies for two temperature radiation diffusion models with significantly varying opacity values. The methods were: block Jacobi, Schur complement and two splitting approaches that split the preconditioner solve into two stages. One splitting method includes the coupling of the radiation and material fields that appears in the matrix diagonal in the first solve, the other method puts this coupling into the second solve. All preconditioning approaches use multigrid methods to invert blocks of the Jacobian formed from the diffusion operator. The Schur complement approach was clearly seen to be the most effective for various values of opacities, for different weightings of the diffusion and energy coupling terms and for tabulated opacities as well. In the case of tabulated opacity values, only the Schur complement preconditioning approach was able to effectively solve the linear systems once the time steps became large. These results were written into a paper submitted to and accepted by the *SIAM Journal on Scientific Computing*.

Boltzmann Solver Accomplishments

We added a time-dependent capability to our steady-state Boltzmann equation solver. This has been based on a generic differential/algebraic equation solver developed at LLNL as part of the *PVODE* solver suite. A scalability study similar to that done for the radiation-diffusion code was done for this code. The problem contained an internal steady state source localized in space at the center of the spatial domain, with Dirichlet boundary conditions, and the time simulation was done until the solution had converged to essentially steady state. All results used 30x30x30 spatial zones with 24 directions per processor, and 1 energy group. The largest problem had over 663 million unknowns.

Table 4. Scalability study for time-dependent Boltzmann code

Processor Topology	NST	Run Time (seconds)	NRE	NLI	Avg. Cost Timestep	R.T. Scaled Eff.	T.S. Scaled Eff.
1x1x1	124	1810.61	228	103	16.60s	--	--
2x2x2	140	2498.38	261	120	17.85s	73%	93%
4x4x4	151	2865.22	283	131	18.97s	63%	88%
8x8x8	166	3378.23	318	151	20.35s	54%	82%
16x8x8	181	3813.68	343	161	21.06s	48%	79%

(NST = # of time steps, NRE = # of function evaluations)

Table 4 summarizes the results of the study. While the number of time steps degraded somewhat, the current implementation scaled extremely well when comparing the average cost of a time step. As this run is also a time dependent simulation running to a steady state solution, we simply may not have run the time simulation long enough to see the scalability in the number of time steps. The preconditioner used in this run does not take scattering into account, but the code can employ diffusion-based DSA preconditioning on an energy group basis combined with a block-based (in energy group) Gauss-Seidel preconditioner. The code is also capable of performing first scatter solutions for problems with point sources, both constant and pulsed in time. Using a model of the National Ignition Facility (NIF) target bay, we performed steady state and time dependent simulations on the LLNL Compaq Tera Cluster. The purpose of these calculations was to simulate the flux of fusion neutrons discharged from the NIF target chamber during an actual experiment. Similar calculations are used to calculate yearly dose rates for workers servicing equipment in the target bay. These preliminary computations were carried out on 128 CPU's of the Tera Cluster (200 million unknowns). For the steady state problem, a constant neutron source at the center of the NIF sphere was assumed, while for the time-dependent problem a neutron pulse originating at the sphere center was modeled. Figure 1 shows the model of the NIF target bay, along with pictures of the scalar flux first-scatter and steady-state solutions, and a snapshot of the time dependent pulsed solution.

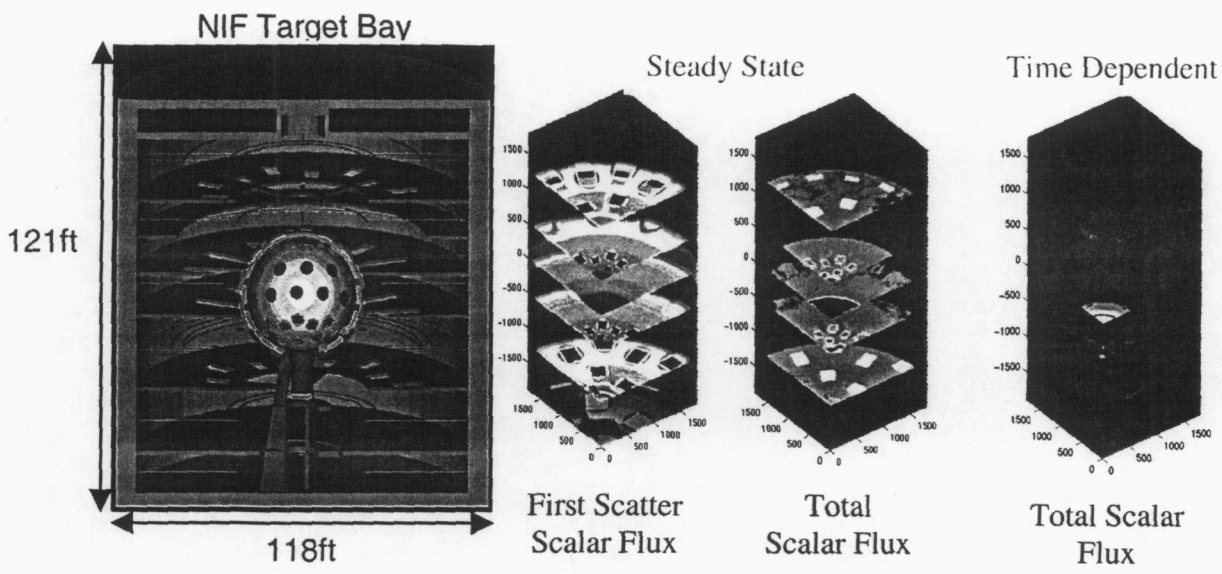

Figure 1

Using our *Harmonic Projection* algorithm, which obtains a spherical harmonics solution by solving a modified discrete ordinates system, we performed a full-system run of our steady state Boltzmann code on the ASCI Blue Pacific SST. The purpose of this calculation was to simulate the flux of fusion neutrons that comes out of the NOVA target chamber. The fusion neutrons can be very penetrating when they emerge from the target chamber because they are born at a very high energy (14.1MeV), and can be dangerous if not absorbed in a shield. This calculation allowed us to show unprecedented detail in the total neutron scalar flux distribution, and is

arguably the largest deterministic transport calculation ever performed. We also demonstrated the ability of our harmonic projection method to give a solution without ray effects on a problem with widely varying spatial scales (4 orders of magnitude) and material properties (14 orders of magnitude). The source of neutrons was a point source at the center of the hohlraum in the target chamber. Figure 2 displays the complex geometry involved in the description of the NOVA target chamber. Isosurfaces in Figure 3 display a cut-away view of the interior of the chamber. In particular, the target assembly is shown along with the interior geometry of the chamber. The colors on the isosurfaces represent values of the total neutron scalar flux, with red denoting the regions of highest flux and blue the lowest. The spatial mesh used roughly 160 million spatial zones, and there were 23 energy groups, with P_1 scattering in each group (requiring 4 moments per zone), for a total of 15 billion unknowns. The multigroup solution took roughly 27 hours on the S and K sectors of the SST, using 960 nodes and 3,840 processors (with OpenMP threads). This run also gave us the opportunity to investigate the scalability of our methods on problems requiring thousands of processors and billions of unknowns, and demonstrated a lack of scalability of our iterative solution method when using the harmonic projection option.

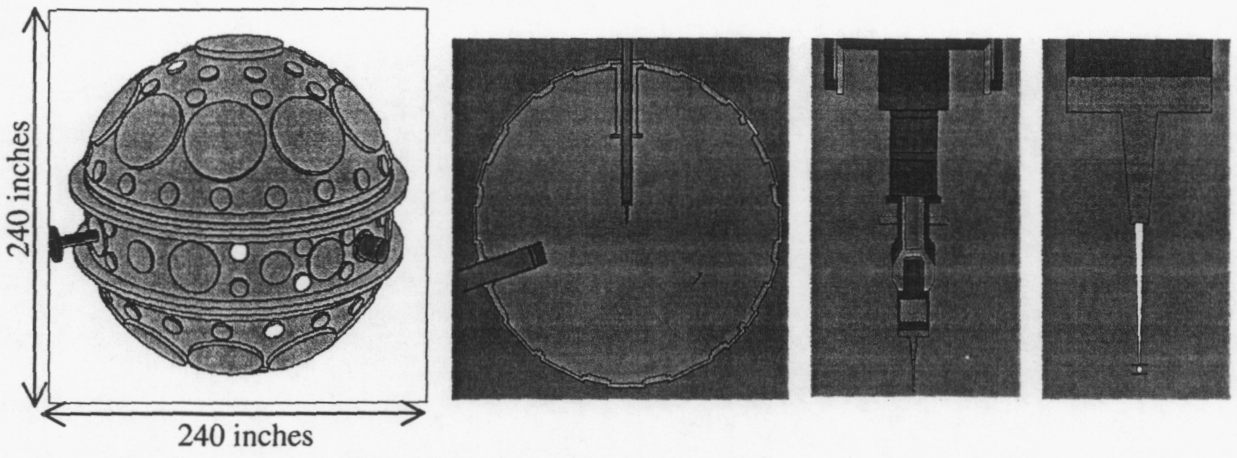

Figure 2. NOVA Target Chamber Geometry. The pictures from left to right show the increasing spatial detail.

A second run of the steady state Boltzmann code on the same problem employed more than 151 million zones with over 27 billion unknowns. This run used the discrete ordinates approximation and OpenMP threads, and took 4 hours to solve on 4,992 processors of the LLNL ASCI SST, running on 1,248 nodes with 4 threads per node. Figure 4 compares the differences between solutions obtained using the spherical harmonics solution approach and this second run using discrete ordinates. Due to the highly localized source in this problem, the discrete ordinates solution is polluted with unphysical ray effects. The use of methods that eliminate or greatly mitigate ray effects is important in many applications at the laboratory.

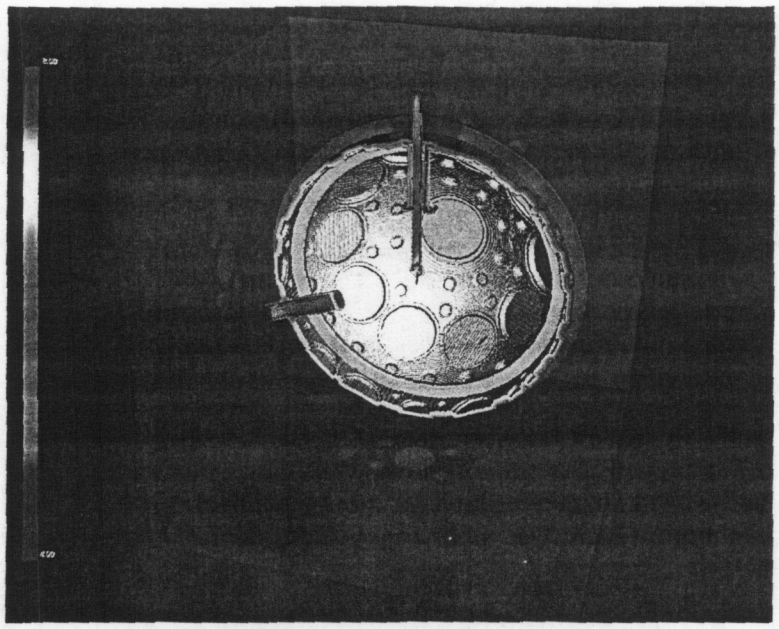

Figure 3. NOVA Target Chamber Simulation

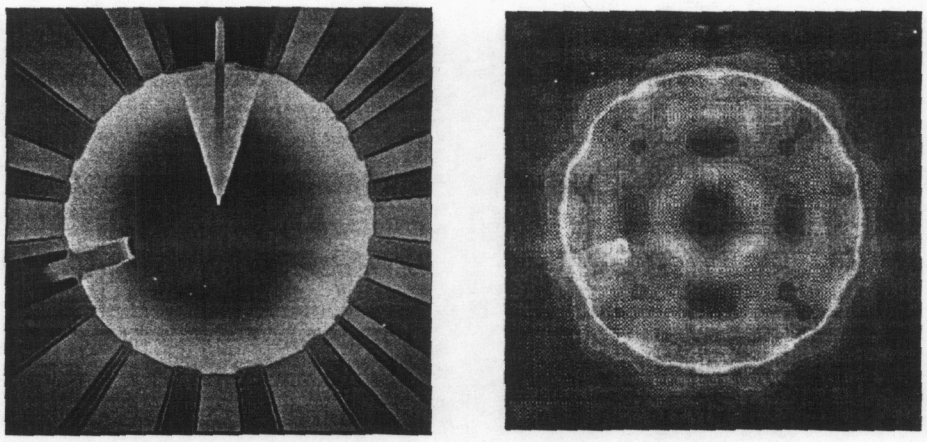

Figure 4. Comparison of the scalar flux in the NOVA target chamber problem obtained using spherical harmonics (left) and discrete ordinates (right).

RETURN TO THE LABORATORY

As we noted above, the modeling of photon and neutron transport is an important capability for a number of Laboratory programs, comprising a significant fraction of the computational cost in many multi-physics simulations. We are collaborating closely with researchers in the Defense and Nuclear Technologies (DNT) Directorate on methods for neutron and radiation transport. There is currently much interest in the methods we have developed for radiation and neutron transport among our collaborators in DNT.

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